Transfer matrices and lattice fermions at finite density

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I discuss the connection between the Hamiltonian and path integral approaches for fermionic fields. I show how the temporal Wilson projection operators appear naturally in a lattice action. I also carefully treat the insertion of a chemical potential term.

It is a pleasure to contribute to this volume honoring Kurt Haller. Kurt and I have long shared strong interests in the connection between Hamiltonian and Lagrangian formulations of field theory. We have both extensively investigated the "temporal gauge" with hopes of gaining insight into non-perturbative phenomena in gauge theories [1]. Topological tunnelling issues in the Hamiltonian formalism have been entwined with much of this activity. While Kurt has emphasized the continuum formulation, for me many of these ideas have become increasingly involved with lattice issues. Actually my first paper on the temporal gauge concerned the lattice [2], showing the connection between the Lagrangian formulation of Wilson and the Hamiltonian formulation of Kogut and Susskind.

Here I expand on some of these old relations between the Hilbert space approach and path integrals, with an emphasis on the complications arising with anticommuting fields. My initial paper on the transfer matrix concentrated on gauge fields and was rather terse with fermions [2]. Later I returned to these issues, pointing out how the Wilson projection operator formalism [5] naturally arises [3]. Here I reconstruct that argument in a more pedagogical manner, adding comments on how a chemical potential, representing a non-zero baryon density, most naturally appears in a fermionic path integral.

Anticommutation is at the heart of fermionic behavior. This is true in both Hamiltonian operator formalisms and Lagrangian path integral approaches, but in rather complementary ways. If an operator $a^\dagger$ creates a fermion in some normalized state on the lattice or the continuum, it satisfies the basic relation

$$[a, a^\dagger]_+ \equiv aa^\dagger + a^\dagger a = 1. \tag{1}$$

This contrasts sharply with the fields in a path integral, which all anticommute

$$[\chi, \chi^\dagger]_+ = 0. \tag{2}$$

The connection between the Hilbert space approach and the path integral appear through the transfer matrix formalism. For bosonic fields this is straightforward, but for fermions certain subtlies arise, related to the so called "doubling problem."

To be more precise, consider a single fermion state created by the operator $a^\dagger$, and an antiparticle state created by another operator $b^\dagger$. For an extremely simple model, consider the Hamiltonian

$$H = m(a^\dagger a + b^\dagger b) + \mu(a^\dagger a - b^\dagger b). \tag{3}$$

Here m can be thought of as a "mass" for the particle, and μ represents a chemical potential. What I want is an exact path integral expression for the partition function

$$Z = \mathrm{Tr}\, e^{-\beta H}. \tag{4}$$

Of course, since my Hilbert space has only four states, this is trivial to work out: $Z = 1 + e^{m+\mu} + e^{m-\mu} + e^{2m}$. However, I want this in a form that easily generalizes to many variables, makes the connection with the Wilson projection operator clear, and illustrates how the chemical potential is properly inserted into a path integral.

A path integral for fermions uses Grassmann variables [4]. I introduce a pair of such, χ and $\chi^\dagger$, which will be connected to the operator pair a and $a^\dagger$, and another pair, ξ and $\xi^\dagger$, for b, $b^\dagger$. All the Grassmann variables anticommute. Integration over any of them is determined by the simple formulas

$$\int d\chi\, 1 = 0 \ ; \qquad \int d\chi\, \chi = 1. \tag{5}$$

This determines my phase conventions. For notational simplicity I join individual Grassmann variables into spinors

$$\psi = \begin{pmatrix} \chi \\ \xi^\dagger \end{pmatrix}; \quad \psi^\dagger = \begin{pmatrix} \chi^\dagger & \xi \end{pmatrix}. \tag{6}$$

To make things appear still more familiar, introduce a "Dirac matrix"

$$\gamma_0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{7}$$

and the usual

$$\overline{\psi} = \psi^\dagger \gamma_0. \tag{8}$$

Then we have

$$\overline{\psi}\psi = \chi^\dagger \chi + \xi^\dagger \xi. \tag{9}$$

The temporal Wilson projection [5] operators

$$P_\pm = \frac{1}{2}(1 \pm \gamma_0) \tag{10}$$

arise when one considers the fields at two different locations

$$\chi_i^\dagger \chi_j + \xi_i^\dagger \xi_j = \overline{\psi}_i P_+ \psi_j + \overline{\psi}_j P_- \psi_i. \tag{11}$$

The indices i and j will soon label the ends of a temporal hopping term; this formula is the basic transfer matrix justification for the projection operator formalism.

For a moment I ignore the antiparticles and consider some general operator $f(a, a^\dagger)$ in my Hilbert space. How is this related to an integration in Grassmann space? To proceed I need a convention for ordering the operators in f. I adopt the usual normal ordering definition with the notation $: f(a, a^\dagger) :$ meaning that creation operators are placed to the

left of destruction operators, with a minus sign inserted for each exchange. In this case a rather simple formula gives the trace of the operator as a Grassmann integration

$$\text{Tr} \ : f(a, a^\dagger) : = \int d\chi d\chi^\dagger e^{2\chi^\dagger \chi} f(\chi, \chi^\dagger). \tag{12}$$

To verify, just check that all elements of the complete set of operators $\{1, a, a^\dagger, a^\dagger a\}$ work. However, this formula is actually much more general; with a set of Grassmann variables $\{\chi, \chi^\dagger\}$, one pair for each fermion state, this immediately generalizes to the trace of any normal ordered operator acting in a many fermion Hilbert space.

What about a product of several normal ordered operators? This leads to the introduction of multiple sets of Grassmann variables and the general formula [3,6,7]

$$\text{Tr} \ : f_1(a^\dagger, a) : : f_2(a^\dagger, a) : \ldots : f_n(a^\dagger, a) : =$$
$$\int d\chi_1 \, d\chi_1^* \ldots d\chi_n \, d\chi_n^*$$
$$e^{\chi_1^*(\chi_1 + \chi_n)} e^{\chi_2^*(\chi_2 - \chi_1)} \ldots e^{\chi_n^*(\chi_n - \chi_{n-1})}$$
$$f_1(\chi_1^*, \chi_1) f_2(\chi_2^*, \chi_2) \ldots f_n(\chi_n^*, \chi_n). \tag{13}$$

The positive sign on χ_n in the first exponential factor indicates the natural occurance of antiperiodic boundary conditions. With just one factor, this formula reduces to the previous relation. Note how the "time derivative" terms are "one sided;" this is how doubling is eluded.

This exact relationship provides the starting place for converting our partition function into a path integral. The simplicity of the Hamiltonian allows this to be done exactly at every stage. First I break "time" into a number N of "slices"

$$Z = \text{Tr} \left(e^{-\beta H/N} \right)^N. \tag{14}$$

Now I need normal ordered factors for the above formula. For this I use

$$e^{\alpha a^\dagger a} = 1 + (e^\alpha - 1) a^\dagger a = \ : e^{(e^\alpha - 1) a^\dagger a} : \ , \tag{15}$$

true for arbitrary parameter α. Combining the particles and antiparticles into one matrix equation gives

$$\exp((\alpha + \rho) a^\dagger a + (\alpha - \rho) b^\dagger b) = \ : \exp \left((a^\dagger \quad b^\dagger) \left(e^{\alpha + \rho \gamma_0} - 1 \right) \begin{pmatrix} a \\ b \end{pmatrix} \right) : \ , \tag{16}$$

The -1 in this exponent will cancel the diagonal terms in the exponentials of Eq. (13).

This is all the machinery I need to write

$$Z = \int (d\psi d\psi^\dagger) e^S \tag{17}$$

where

$$S = \sum_{i=1}^{n} \overline{\psi}_n e^{-\beta m/N} e^{-\beta \mu \gamma_0/N} \psi_n - \overline{\psi}_n P_+ \psi_{n-1} - \overline{\psi}_{n-1} P_- \psi_n. \tag{18}$$

Note how the Wilson projection factors of $P_\pm$ automatically appear via Eq. (11) to handle the reverse convention of χ versus ξ in our field ψ. The projection operator formalism is a natural consequence of an exact transfer matrix.

The chemical potential appears simply as an inserted factor of $e^{-\beta\mu\gamma_0/N}$ in the "mass" term. This is not quite in the conventional form [8] since the chemical potential piece is temporally diagonal. However this is actually only a convention, as the factor can be moved to temporal links with a change of variable

$$\Psi \equiv e^{\frac{-\beta\mu\gamma_0}{2N}}\psi. \tag{19}$$

With this substitution, we have

$$S = \sum_{i=1}^{n} \overline{\Psi}_n e^{-\beta m/N}\Psi_n - \overline{\Psi}_n P_+ e^{\beta\mu/N}\Psi_{n-1} - \overline{\Psi}_{n-1} P_- e^{-\beta\mu/N}\Psi_n. \tag{20}$$

If μ were imaginary, this would be precisely the form of a $U(1)$ gauge field on the timelike bonds.

In this discussion I have ignored spatial hoppings. Terms in the action of the form

$$\overline{\psi}\vec{D}\cdot\vec{\gamma}\psi \tag{21}$$

are invariant under this change of variables since γ_0 anticommutes with $\vec{\gamma}$. However, more complicated terms, such as spatial Wilson hoppings, are generally not invariant under this change. This would be a modification of higher order in the lattice spacing for Wilson fermions. These are lattice artifacts, presumably irrelevant to the continuum limit. Thus, it is only a convention whether the chemical potiential is inserted as a matrix valued mass as in Eq. (18) or as a direction dependent link term as in Eq. (20).

If we consider the action as a generalized matrix connecting fermionic variables

$$S = \overline{\psi}M\psi, \tag{22}$$

the matrix M is not symmetric. The upper components propagate forward in time, and the lower components backward. Even though our Hamiltonian was Hermitian, the matrix appearing in the corresponding action is not. With further interactions, such as gauge field effects, the intermediate fermion contributions to a general path integral are generally not positive, or even real. Of course the final partition function, being a trace of a positive definite operator, is positive. However, depending on the order of operations, there can be negative intermediate results. With Monte Carlo methods, this can lead to uncontrollable fluctuations. This is the primary unsolved problem in lattice gauge theory. With no chemical potential term, symmetry between particles and antiparticles results in a real fermion determinant, which in turn is positive for an even number of flavors.

For our simple Hamiltonian, this discussion has been exact. The discretization of time adds no approximations since we could do the normal ordering by hand. In general with spatial hopping or more complex interactions, the normal ordering can produce extra terms going as $O(1/N^2)$. In this case exact results require a limit of a large number of time slices.

In summary, my goals in this discussion were twofold. First a careful transfer matrix treatment makes the Wilson projection operator a natural approach to eliminate temporal

doubling. Second, I have shown explicitly how to insert a chemical potential term in a path integral. It is a convention whether this term appears appears as non-symmetric temporal hoppings or as a matrix-valued effective mass.

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